

# Advanced Fuel Cycle Initiative



Technical Monthly - June 2003

## Systems Analysis

### Transmutation Studies and Integrated Fuel Cycle Modeling

[ALL] A workshop on Transmutation Criteria was hosted by ANL on June 18 and 19. The workshop was attended by participants from ANL, BNL, INEEL, LANL, ORNL, SNL, WSRC, LLNL, and USDOE. The objective of the workshop was to provide a detailed assessment of the current reference flowsheet and to specify material pathways and technical criteria for the AFCI. The criteria discussed included proliferation resistance, repository objectives, uranium disposal pathways, long-lived fission products transmutation, actinide recycle in LWRs, curium pathways, cesium and strontium recovery, transuranics burning, and separations criteria. For each topic, detailed technical presentations, including a proposal and justification for technical criteria, were developed by the meeting participants. The key conclusions and recommendations in each area are documented in the meeting minutes.

[ANL] The *deliverable report* on LWR transmutation schemes was completed. The physics and safety issues for multi-recycle were reviewed. Possible implementation schemes for plutonium and selective minor actinide recycle were described; additional consideration of LWR targets and nonfertile fuel options will be included in the final report.

[BNL] A series of benchmark calculations with MCNP is being pursued to "validate" the initial Series-1 assembly design with Np+Pu MOX. Work on developing detailed MCNP geometry models for an isolated Np+Pu MOX assembly, and a "colorset" geometry with one MOX assembly and 3-UOX assemblies was initiated.

[LANL] A second iteration of benchmarking the

COSI and NFCSim codes was completed. A second set of results were generated to align the NFCSim results more closely, where possible, with the COSI results.

[ANL] Power peaking analyses have been completed for MOX assemblies fabricated with separated Pu or Pu+Np in an environment of fresh, once-, and twice-burned  $\text{UO}_2$ ; this arrangement simulates the MOX assembly being inserted in a typical multiple-batch PWR core loading. For the optimized MOX assembly design (see May monthly) using separated Pu, a peak  $F_{\text{FH}}$  of 1.486 occurs in a neighboring fresh  $\text{UO}_2$  assembly; if MOX is fabricated from Pu+Np, the peak  $F_{\text{FH}}$  is 1.506. In both cases, however, the  $F_{\text{FH}}$  is below the typical PWR core design limit of 1.55. Further suppression of the power peaking may result from the use of  $\text{Gd}_2\text{O}_3$ -poison in the  $\text{UO}_2$  assemblies; this is under investigation.

[ANL] A preliminary evaluation was conducted of transuranic (TRU) containing product characteristics resulting from processing spent LWR fuel to remove cesium, strontium, iodine, technetium, and uranium; in particular, the radiation source and thermal properties were considered. Calculations showed that if the spent fuel is processed after 30 years cooling, there is roughly a factor of two reduction of the peak dose rate 1 meter from the bare waste form, due to the cesium removal. Thermal analyses indicate that removal of short-term heat load (cesium and strontium) may be beneficial for interim storage; however, repository disposal size/concentration would not be reduced because the long-term heat load has not been impacted.

[LANL] The basis for preliminary cost models was completed for reprocessing and fuel fabrication for

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recycling Pu, Pu + Np, Pu + Np + Am, and Pu + Np + Am + Cm in MOX fuel to be burned in Tier 1:

- the reprocessing cost is dictated by additional separations, and
- the fuel fabrication cost is dictated by additional dose.

[ANL] A comparative physics study will be conducted to compare the general transmutation potential of sodium, gas, lead, and LBE cooled systems. This work is being conducted jointly with CEA as part of the collaboration agreement. This month, one-group cross section data for a broad spectrum of actinides was generated for the sodium-cooled case. Material compositions from a burner configuration were employed, and data was generated for both metal and oxide fuel. The spectrum is softer with oxide fuel, and the fission/absorption ratios are slightly reduced.

[ANL] Work was initiated on the design and evaluation of a gas-cooled fast reactor (GFR) transmutation core, starting with the high conversion ratio core designs being evaluated in the Generation IV program. In addition, GFR design data supplied by CEA was reviewed.

[BNL, ANL] The activity on Reduced Moderation Water Reactor (RMWR) was started this month. One-group cross sections [absorption, fission, and (n,2n)] were obtained at room temperature with MCNP for a Reduced Moderator Water Reactor (RMWR) pin-cell based on information provided by JAERI. The one-group data will be used in a similar collaborative evaluation of LWR Transmutation Options via the D-factor approach. Additional information on the current assembly configuration for the RMWR, including dimensions and enrichment distribution has been requested from JAERI. An evaluation of the adequacy of thermal reactor lattice codes for this design is ongoing. Preliminary results suggest that a more robust lattice capability encompassing features of thermal and fast lattice codes might be required.

[ANL] Thermal analyses of the Yucca Mountain

Repository were conducted to investigate the effect of removing uranium and the fission products cesium and strontium from the spent fuel. Results indicate that the benefit of such a strategy is limited to allowing a shorter preclosure ventilation time, that would permit closing the repository sooner. Although the waste packages may be smaller, the overall size of the repository is not changed, with the decay heat from the remaining actinides still providing the limiting thermal conditions in the repository.

[ANL, LANL] A paper on the Phase 1 nonproliferation activities was presented at the IAEA Conference on Innovative Technologies for Advanced Fuel Cycles, held in Vienna.

[ANL] The compact configuration with conversion ratio ~0.25 was chosen as the *reference low conversion ratio fast reactor design*; the metal fuel enrichment is roughly 50% TRU/HM with FFTF-size pins. This point design is more aggressive than the FY02 high leakage concept; it has a significantly higher power density and less favorable reactivity coefficients. Detailed SAS4A reactivity worth tables were generated for use in a detailed safety assessment.

[ANL] The deliverable *report* describing system design and fuel cycle analysis of the low conversion ratio fast reactor concept was completed.

[ORNL] Completed initial assessment for Pu and minor actinide transmutation potential for candidate LWR fuel cycles.

## Repository Impacts

[LLNL] Participating (in support of DOE-RW) in a NEA Working Group: "Expert Group on the Impact of Advanced Nuclear Fuel Cycle Options on Waste Management Policies". The working group held its second meeting June 16, 17 at NEA in Paris.

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# Separations

## Advanced Aqueous Separations

**[ANL] AMUSE Code Development** – AMUSE was enhanced to generate a flowsheet where distribution coefficient (D) values are defined by the user. If a flowsheet needs to be designed with a solvent not incorporated into AMUSE, the user can specify the D values for the components, and a flowsheet can be generated. This option was available in a far less user-friendly mode in the GTM, but had not been updated in AMUSE. Due to newly established Applied Technology requirements, a version of AMUSE, named AMUSE-Lite, was developed to allow continued development of the graphic user interface and optimization codes at UNLV. This version contains appropriate input and output functions, but the technically important files that predict chemical behavior are removed.

**[ANL] UREX+ Laboratory-Scale Hot Demonstration Feed Preparation** – Approximately 1.2 kg of irradiated nuclear fuel from Big Rock Point Reactor was cut into one-inch sections in the alpha/gamma hot cell facility in building 212 and shipped to the shielded cell facility in building 205. The fuel was unpacked and placed in our cell in preparation for dissolution. The chopped fuel was removed from the shipping container and examined. Three separate charges will be selected each containing about 400 g of fuel.

**[ANL] Cs/Sr Separation** – Dispersion tests were completed for the CDC-PEG solvent (produced by INEEL) with simulants of the aqueous process streams to be used for the INEEL-designed CDC-PEG process. The dispersion numbers for all solutions indicated excellent or very good separation of the phases. One-stage hydraulic testing was also performed using the new centrifugal contactor that will be installed in the shielded cell facility. Good hydraulic performance was found for total flow rates up to 60 mL/min for each section.

**[ANL] Rare Earth/Actinide Recovery Process Development** – A batch-contact flowsheet was

generated using AMUSE to simulate the TRUEX process to be demonstrated. The Pu/Np raffinate was the assumed feed. The extraction and each of the three scrub stages were simulated with up to three batch contacts. The O/A for each section was varied until concentration levels in the equilibrated effluent approached those obtained for the full process simulation. Based on this flowsheet, a series of batch contacts were performed verified the efficacy of the flowsheet, especially that precipitation of lanthanide oxalate salts will be avoided.

## **[ANL] Am/Cm Separation Process Development**

- Purification of Cyanex 301 continued this month with approximately 300 g of dry white crystals purified from the commercial product, which is contaminated with inorganic and organic impurities. Distribution ratios for  $^{241}\text{Am}$  and  $^{152}\text{Eu}$  at tracer levels were measured for two batches of material (the second with superior purification). The purified Cyanex 301 was dissolved in a solution of tributyl phosphate and n-dodecane. Both batches extracted  $^{241}\text{Am}$  with a high D value ( $>340$  for the first batch and 310 for the second). However, the  $^{152}\text{Eu}$  D values were higher than wanted for processing (10.7 and 4.8, where 0.1 or less is required). Studies are planned to determine (1) the level of impurity by adding micro quantities of natural Eu up to its expected concentration in the feed, (2) if this level will cause difficulty in meeting process goals for the demonstration, and (3) whether further purification of the Cyanex 301 is necessary. Literature studies have shown that, for purified Cyanex 301, higher lanthanide concentrations drop their distribution ratios considerably.

**[ORNL] SANEX Process Development** - The testing of extractants for the group separation of the actinides and lanthanides continued with initial testing of the BTP extractant, 2,6-bis(5,6-di-ethyl-1,2,4-triazin-3-yl)-pyridine. Promising americium distributions ( $D(\text{Am}) = 6-10$ ) were obtained with nitric acid concentrations in the range 0.25 to 0.75 M with corresponding americium/europium separation

## ***Separations continued***

factors (SF) of 100-120. In parallel with the BTP experiments, the bis(chlorophenyl)-dithiophosphinic acid/Cyanex® 923, the Cyanex® 301/Cyanex® 923, and the di-2-ethylhexyl phosphoric acid (HDEHP) systems were evaluated for comparison purposes with the initial dithiophosphinic acid data and the BTP extraction data. The results of these tests yielded comparable results (SF = 35) for the dithiophosphinic acid system and low distribution and separation (SF = 3) for the Cyanex® 301 system at 0.01 M nitric acid concentration. The preliminary data from the extraction of both the actinides and lanthanides in the HDEHP system followed by subsequent stripping of the actinide fraction is being evaluated.

**[ORNL] UREX+ Co-Decontamination Solvent Extraction Hot Test** - In preparation for the hot tests, two of the three mixer-settler banks were removed from the equipment rack for repair (in the hot cell) of leaking gaskets and refurbishment of the drive gears for the stirrer. After reinstallation and leak testing, an ~ 8-hour test operation was performed using depleted uranium as the spent fuel simulant. All operations were satisfactory. All of the reagent addition flow controllers were re-calibrated for the flow rate ranges that will be used in the hot tests.

**[INEEL] UREX + Engineering-Scale Experiment** - The 60% design review package of the preconceptual design being completed by Washington Group International was issued for review and the 60% design review meeting is scheduled at the INEEL on June 26<sup>th</sup> and 27<sup>th</sup>. The High-Level Functions and Requirements document has been revised to incorporate changes in the flowsheet requirements and is being reissued for approval. A document detailing the potential uses for the TAN-607 facility has been drafted and an initial review completed. This document will be used to attempt to obtain concurrence on a path forward that will allow the UREX + ESE to use this facility. A Mission Need Statement has been drafted

and internal INEEL reviews are being conducted. A Technical Strategy Plan that details bench scale testing needs and the UREX + ESE testing requirements has been drafted, reviewed and comments are being incorporated. It will be issued for final review and comments in July.

### **[INEEL] Cs/Sr Extraction Process Development**

- Based on the results to date of laboratory testing of a chlorinated cobalt dicarbollide (CCD)/polyethylene glycol (PEG) based solvent extraction process for the separation of Cs and Sr from dissolved LWR fuel, a flowsheet was provided to ANL-E to support flowsheet testing planned for this summer. The flowsheet consists of 8 stages of extraction, 4 stages of 3 M HNO<sub>3</sub> scrub, 10 stages of 100 g/L guanidine carbonate; 20 g/L DTPA strip, and 2 stages of nitric acid wash. Approximately one liter of the CCD/PEG solvent was prepared and shipped to ANL-E to support hydraulic testing in the contactors prior to installation in the hot cell. Additionally, two liters of the phenyltrifluoromethyl sulfone diluent has been synthesized and is being shipped to the INEEL. This diluent will be used to make up 1.5 liters of CCD/PEG solvent for use in the flowsheet testing at ANL-E this summer.

### **Pyrochemical Separations**

**[ANL] Oxide Reduction Process Development** - Analysis of the data from the second high-capacity reduction experiment revealed that the cell operated with improved current efficiency and the on-line oxygen measurement system can be effectively used to monitor the status of the reduction process including determining the termination point of the reduction run.

**[ANL] Anode Materials Development** - Several composite ceramic anodes, constructed with low-cost binder materials, were evaluated in the polarization test cell. Each anode performed well and showed no visible signs of chemical attack. The anodes will be subjected to more severe test conditions to assess their viability.



## ***Separations continued***

### **Engineered Product Storage**

**[LANL] Technetium Product Preparation for Storage/Transmutation.** A technetium recovery method for the UREX technetium product stream was further evaluated. This method requires prior removal of the nitric acid from the UREX Tc product solution, followed by re-dissolution in water, cation exchange to remove impurities, making the solution basic, adding  $\text{BH}_4^-$ , and generating technetium metal by a slow addition of acetic acid. The product is a metal powder that stages the technetium for conversion to a solid metal form for storage or transmutation. The factors controlling the precipitation process have been investigated in more detail. Removing the nitrate from the system is critical. The presence of nitrate appears to give  $\text{TcO}_2$  or a mixed  $\text{TcO}_2$ /metal product. Chemical denitration with sucrose, without any iron catalyst, was slow. Excess sucrose used in the denitration reaction interferes with the technetium metal precipitation by preventing the metal from coagulating. The black suspension (colloid) of technetium metal does not centrifuge out after 20 minutes at 4000 rpm. Based on these results, distilling off the nitric acid appears to be the best route for nitrate removal from the system. Most of the nitric acid (90-95%) can be distilled off readily, but removing the acid to near dryness to greatly reduce the nitrate content of the redissolved salt can lead to volatilization of technetium, probably as  $\text{Tc}_2\text{O}_7$ . It will be necessary to limit the temperature of the acid distillation at this point. Retention of technetium with careful temperature control is >95%.

### **Spent Fuel Treatment Facility Design**

**[ORNL] Deployment Options** - Efforts supporting preparation of the Deployment Plan continued. Review of the draft plan indicated the need to add “timing of deployment” as a significant parameter for startup of the spent fuel treatment facility (SFTF). Examination of this parameter indicates that delaying deployment can have considerable consequences on the ultimate lifetime of the Yucca Mountain repository.

Using the shipping schedule, a timeline showing the percent of YM authorized capacity that can be consumed by unprocessed spent fuel, assuming immediate emplacement, was prepared.

Implementation of a treatment facility in 2015 results in ~16% of the repository being consumed with unprocessed material. This is unavoidable, unless interim storage is implemented at YM, because a plant cannot be built and placed on-line any earlier than 2015. However, this small fraction (~16%) of the repository does not greatly degrade the repository life-span if spent fuel treatment is deployed to reduce the fill-rate of the repository from 2015 forward. Delays until 2020 result in ~40% of the repository having been consumed, greatly increasing the risk that a second repository will be required. Delays until 2030 result in ~88% of the repository being consumed and *guarantee* that a second repository is required (or a very high price paid to retrieve the material and reprocess it along with material that continues to arrive at YM with either 2 large plants or one very large plant to keep-up with both material streams).

**[ORNL] Spent Fuel Characteristics** - Data from ORIGEN calculations were used to calculate the spontaneous neutron generation rate, gamma/photon rate, and gamma energy rate for the transuranium (TRU) products, Np, Pu, Am, and Cm from 2000 MTIHM of spent fuel. Charts were prepared showing the change in these emissions with fuel age and fuel burnup.

**[INEEL] Spent Fuel Treatment Facility (SFTF) Design Support** - All comments from the Separations Working Group members have been incorporated into the SFTF High-Level Functions and Requirements (F&R's) for the facility. Final review and approval will be obtained and the F&R's will be issued in July.

**[WSRC] SFTF Deployment Planning** - The Separations Deployment Options activity team continues to evaluate various strategic approaches

## ***Separations continued***

for the deployment of a Spent Fuel Treatment facility. Several “white paper” documents were generated for team discussion during the past month. These documents pertain to justification for the SFTF capacity and spent fuel feed age criteria. In addition, a separate summary was drafted outlining factors in support of an expedited SFTF startup date. These items will be discussed and refined within the working group in order to incorporate consensus agreements into the deployment strategy. The latest working draft of the SFTF Deployment plan was issued for review to members of the Separations Deployment activity team. In addition, the latest version of the planning matrix plus a graphical recommendation for a nominal SFTF processing rate was included in order to gain team member concurrence. The key issues for continued development remain capacity and timing of the SFTF. The general conclusions from the Transmutation Criteria Workshop are being incorporated into the overall planning.

### **Advanced Process Development**

**[LANL] Actinide Crystallization Process.** The first series of bench-scale uranyl nitrate crystallization tests was completed. Decontamination factors for 6-9 fission product elements were measured and were generally in the range of 30-100. This is similar to what has been observed in bench-scale crystallization reports in the literature. The loop crystallizer assembly is nearly complete for testing with non-radioactive materials. The tests in the loop crystallizer will use water, nitric acid, and salts such as calcium or cerium nitrate to test the operation of the unit. The operational functions include:

- a) feed preheat and flash system.
- b) overhead vapor condensing and vacuum system.
- c) crystallization loop circulation using only flashed vapor (no impeller)
- d) flow and density measuring instruments.
- e) physical operation of the crystal filters and liquid removal.

f) fines removal system and fines recycle.

### **EBR-II Spent Fuel Treatment**

**[ANL] EBR-II Blanket Processing** - Seventy-one kilograms of heavy metal from blanket material were processed in the Mark-V electrorefiner (ER) during the month of June. Processing the blanket fuel serves to increase the plutonium content in the salt in support of transuranic (TRU) recovery tests. A total of 334 kilograms of fuel has been treated in FY03.

**[ANL] TRU Recovery with the Liquid Cathode** - Qualification testing of the Liquid Cadmium Cathode (LCC) handling equipment was completed in the Fuel Conditioning Facility (FCF) Mock-up Area. Two additional items of handling equipment were identified during the testing and they are being designed. The qualification test procedure for operation and maintenance of the LCC assembly itself was approved and the testing was initiated by Mockup Area personnel. A test was performed in the FCF cathode processor with 27.2 kg of cadmium and 1.4 kg of LiCl-KCl eutectic salt to simulate LCC operations in terms of processing conditions. The test was successful. More than 99% of the cadmium was recovered in the receiver crucible.

**[ANL] Advanced Electrorefiner Development** - Concept layouts for the Planar Electrode Electrorefiner (PEER) prototype module were completed. Detailed design was initiated of the cover and heat shield assembly, which will be installed on the Mk-III ER well in the glovebox facilities in Illinois and interface with the PEER module itself. A design review of the PEER Cover Assembly was completed.

**[ANL] TRU Recovery by Electrolysis** - Calibration of the anode positioning system and crucible volume of the advanced U/TRU recovery system is complete. Preparations for transferring the system into the hot glovebox are underway. The reference electrode, a key component of the data acquisition and equipment control system, is being fabricated.

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## ***Separations continued***

### **[ANL] Demonstration of PYROX Process -**

Qualification of the electrolytic reduction process with unirradiated depleted uranium oxide fuel in the modified Hot Fuel Dissolution Apparatus (HFDA) has been completed. Approximately 40 g of  $\text{DUO}_2$  was reduced to metal in a qualification run this month. The fuel basket has been sectioned and submitted for chemical analysis to determine the extent of reduction of uranium oxide to uranium metal. Meanwhile, the HFDA is being readied for the next electrolytic reduction run with spent oxide fuel. The milestone "Complete Oxide Fuel Preparation for the Laboratory-Scale PYROX Demonstration," was completed on June 16, 2003. This was slightly ahead of the scheduled date of June 30, 2003. Chemical and radiochemical analyses were completed this month to sufficiently characterize the fuel prior to its introduction into the electrolytic reduction process. Preliminary design criteria for an engineering-scale electrolytic reduction process have been drafted and routed for review. These criteria will form the basis from which pre-conceptual engineering-scale PYROX equipment layouts may be developed.

### **[ANL] Increased Throughput Cathode Processor**

- The milestone "Complete Mockup Qualification Testing of the Larger Capacity Cathode Processor Equipment," was completed on June 3, 2003. This date was well ahead of the scheduled date of June 30, 2003. The new CP equipment consists of internal components and the associated handling fixtures to increase the batch size for depleted uranium product from the Mk-V electrorefiner. The internal components include a process crucible that has forty percent more useable volume.

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## **Integration**

[LANL] We organized the “Materials Modeling and Simulations for Nuclear Fuels” Workshop, June 9-10, 2003, Santa Fe, New Mexico. The meeting was attended by 50 participants, had an international component (8 participants, representing UK, Sweden, and Turkey) and a good participation from universities (9 external and 5 students currently working at LANL). The workshop facilitated a fruitful exchange of ideas and results and generated numerous proposals for scientific collaboration.

[NTD] Based on the input received from various organizations during the FDWG meeting, the NTD presented to DOE a prioritized list of fuel development tasks for FY04 during the NTD meeting on June 25-26 in Washington D.C.

[NTD] A white paper is written on a proposed vision, objectives and quantitative goals for the AFCI program. The white paper is discussed with the other NTDs in the transmutation criteria meeting held in Chicago, on June 17-19, 2003. The white paper also is presented to DOE AFCI staff in Washington D.C. on June 25-26, 2003.

[NTD] The NTD presented the AFCI fuel program in the Fuels and Materials modeling workshop held in Santa Fe on June 9-10, 2003.

[NTD] Meeting minutes of the third FDWG meeting, held in Idaho Falls, on May 21-22, 2003, is published.

## **Series One Fuels Design, Specifications and Analyses**

[WSRC, ORNL] WSRC issued “Evaluation of Initial Market for MOX from Recycled Commercial Spent Nuclear Fuel”. This report reviewed the potential market for Series 1 MOX utilizing the baseline class of reactors being evaluated by the Systems Analysis Working Group. Detailed technical review on the report was provided by ORNL.

[WSRC] Work continued on the Series One Fuel Deployment Plan.

## **Series One Fuel Development & Fabrication**

[LANL] The first oxide test pellets for the LWR-1 experiment have been fabricated. The density was lower than the specification, and further developmental tests are being conducted.

[LANL] The ionic conductivities for nonstoichiometric ceria were calculated in an extended range of temperatures (700 – 1500°C) and oxygen pressures (1-10<sup>-30</sup> atm). The results were related to oxygen diffusivities and a good agreement with previously reported data was obtained. Work is being conducted to extend this method and to adapt the numerical code for UO<sub>(2-X)</sub> and PuO<sub>(2-X)</sub> systems.

[LANL] A procedure has been developed suitable for He bonding of fuel pins for the LWR-1 insertion. The weld procedure met visual inspection, metallographic examination and leak testing requirements. Radiographic examination is pending. Final process qualification and utilization for the LWR-1 pins will occur in July, 2003.

## **Series One ATR Irradiation Experiments**

[INEEL] All initial TRA required documentation for LWR-1 was prepared and submitted.

[INEEL] The Project Execution Plan for LWR-1 was initiated.

[INEEL] Initial physics analysis started based on HUD1 material. The three fuel compositions were supplied by LANL.

## **Series Two Fuel Design Specification and Analyses**

[ANL] A member of the AFCI ANL-W Fuel Development Team attended the AFCI Transmutation Criteria Workshop.

[ANL] A milestone was met with the issuance of the



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program document: Metallic Fuel Testing Requirements.

### **Series Two Nitride Fuel Development**

[LANL] All the non-fertile and low-fertile nitride pellets for the AFC-1AE test have been fabricated.

[LANL] Shipping containers (with improved design) that will be used to ship the nitride pellets to Idaho have been completed.

[LANL] The first-principles database for the modified embedded atom model for AmN was extended to include the B2, L12, and C1 (both Am<sub>2</sub>N and AmN<sub>2</sub>) structures. These additions will not be used in the fitting procedure, but rather as quality checks: if the fitted model gives results for the additional structures in good agreement with our first-principles values then we know we have a model with good transferability. All calculations were performed using the same method as for the pure americium and original AmN cases, i.e., a self-consistent full potential linear muffin-tin orbital method based on the local spin density approximation.

[LANL] Calculations of phase stability in the U-N and Pu-N systems revealed the nonstoichiometry of the UN and PuN compounds. The calculation of the complete phase diagram relies on the models of the thermodynamic properties of the liquid. Models for the free energy of the liquid PuN and UN, based on the knowledge of the partial pressure of N over the two phase region (liquid + compound) have been developed and will be incorporated in the phase diagram calculations.

[ASU, LANL] The presence of well-defined facets in green ZrN powder pellets found during SEM examination indicates that powder compaction is the main mechanism leading to the presence of a crystallographic texture in both green and sintered samples. Quantitative image analysis of fracture surfaces indicates that the cleavage facet area (21.4%) on the

radial plane is about twice as large as that (11.3%) on longitudinal plane after heat treatment. This provides quantitative evidence linking the amount of cleaved particles to fracture toughness anisotropy.

[IC, LANL] Convergence of quantum mechanical (QM) calculations with respect to model parameters has been achieved. The QM calculations predict structures and energies of ZrN-TiN solid solutions as a means to evaluate the reliability of the UN-ZrN simulations. Results for the series of ZrN/TiN compositions (stoichiometries) are consistent with a positive deviation from an ideal solid solution model (that is, they do not follow a simple rule of mixtures). This will have important implications for phase diagram predictions.

### **Series Two Metallic Fuel Development**

[ANL] A casting plan and schedule to satisfy the July milestone for AFC-1F alloys casting was developed.

[ANL] The depleted uranium (DU), enriched uranium (U), Pu, Np and Zr feedstocks required for fabrication of AFC-1F casting were transferred to and sectioned in the Analytical Lab and Casting Lab according to casting plan. Pu/Am feedstock was sectioned.

[ANL] Np feedstock was thermally treated to reduce oxide content. Chemical analysis on the thermally treated Np feedstock indicated oxygen contamination was reduced by about one half to about 2500 ppm.

[ANL] Two of the low-fertile, actinide-bearing metallic fuel samples for AFC-1F were fabricated.

[ANL] Two heat treated (650°C, 200 hrs.) fuel-cladding chemical interaction (FCCI) fuel alloy-422 steel diffusion couples (MB: Pu-10Np-40Zr and MC: Pu-12Am-40Zr) were prepared (cut, ground and polished) and transferred to the EML for SEM study.

[ANL] SEM studies on two fuel alloy-422 steel

## ***Fuels continued***

diffusion couples (ME: Pu-40Zr and MD: Pu-10Am-10Np-40Zr) were completed. No indication of liquid phase formation was noted and no low melting Fe containing phases were observed.

[ANL] A low-fertile metallic alloy (FA: 35U-35Pu-30Zr) was prepared (ground and polished) for SEM study.

[ANL] XRD measurements on low-fertile metallic alloy (FA: 35U-35Pu-30Zr) specimens were completed.

[ANL] The final report for the as-cast non-fertile AFC-1B and -1D alloys thermal analysis studies was completed and issued in fulfillment of the WBS deliverable on June 20, 2003.

### **Series Two Advanced Fuel Forms**

[LANL] Work was initiated to assess the processability and stability of ruthenium aluminide (RuAl) in contact with nitrides and oxides at elevated temperatures. In preparation for this assessment, RuAl was synthesized from the melt and -200 mesh powder was prepared from the RuAl stock. Initial evaluation of cold press/sinter parameters was begun.

[LANL] Particle size characterization and coating work for the micro-structured fuels. Detailed progress is patent-sensitive and is not included here.

### **Series Two ATR Irradiation**

[INEEL] AFC-1B and AFC-1D test assemblies and two dummy capsules were successfully installed into the ATR east flux trap in support of the Advanced Fuel Cycle Initiative. This accomplishment resulted in meeting a level 3 milestones for the AFCI Project.

[ANL] Radiographs of the nitride rodlets that were settled and bonded were evaluated. Development of the settling and bonding procedures continued.

[ANL] The laser flash diffusivity instrument vendor

was visited and the instrument tested and checked out for delivery.

[ANL] The document titled "*Fabrication Control Plan for the AFC-1Æ and AFC-1F Capsule Irradiations in the ATR*" (W7520-0533-ES-00) was completed and submitted to LANL for review and signature. The references and drawings of the document were compiled.

[ANL] The document titled "*Fuel Test Specimen Specification for the AFC-1 Æ Low-Fertile Fuel Capsule Irradiation in the ATR* (W7520-0553-ES-00)", was completed and submitted to LANL for review and signature. This document covers the encapsulation of nitride fuel pellets at ANL-W.

[ANL] Four cadmium-containing baskets for use in the AFC-1B,D fuel experiments were supplied to the ATR. Two dummy stainless steel capsules to serve as replacements for the missing AFC-1A,C nitride fuel tests were also supplied to the ATR.

[ANL] The AFC-1B,D non-fertile metallic fuel experiment capsules were shipped from ANL-W to the ATR on June 4 and began irradiation.

[ANL] The AFC-1Æ and -1F final experiment description and design and data package was initiated.

[INEEL] The AFC-1 Experiment Safety Assurance Package was finalized and approved. This accomplishment resulted in meeting a level 3 milestone for the AFCI Project.

[INEEL] As-run physics analysis for AFC-1B and AFC-1D during the first 21 days of Cycle 131A was performed and documented.

[INEEL] The reactor Primary Coolant System (PCS) was sampled for cadmium each Monday. No increase of cadmium concentrations was detected.

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[INEEL] Preliminary physics analysis for AFC-1Æ, AFC-1F and GFR Materials was initiated.

[INEEL] Preparation of the Experiment Safety Assurance Package for AFC-1Æ, AFC-1F and GFR was initiated.

[INEEL] AFC-1B and AFC-1D test assemblies were received and inspected at the TRA facility.

[INEEL] The AFC-1B and AFC-1D Test Plan was approved, finalized and distributed to DOE and the Fuels Working Group Committee. This resulted in meeting a level 3 milestone for the AFCI Project.

### **Series Two FUTURIX Irradiation**

[ANL, LANL] Plans are progressing for a delegation of CEA fabrication engineers to visit LANL and ANL-W on the week of July 21<sup>st</sup> as part of the process to qualify the site to fabricate the experimental metallic and nitride fuels for the FUTURIX test.

***For more information on Fuels contact Kemal Pasamehmetoglu: (505)667-8893***

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# Transmutation

## **PHYSICS**

### **Cross-Sections**

[ANL] A set of sensitivity coefficients has been generated for the TRAPU-2 and TRAPU-3 irradiation experiments using a simulated adjustment of cross sections.

[ANL] A new evaluation of Am-241 nuclear data was completed. Fission, (n,2n), and (n,3n) reaction cross sections as well as multiplicities for production of Am-242 in the metastable state, were updated by taking into account new experimental data available.

[ANL] A technical paper concerning iron and nickel isotopes, entitled "Neutron-Induced Hydrogen and Helium Production from Threshold to 100 MeV," was prepared and presented at the ANS AccApp'03 Conference (San Diego).

[ANL] Assembly and characterization of thicker CsI(Tl) stopping detectors continued in preparation for next month's experimental runs at LANSCE.

[ANL] Initial electroplated chromium foil was tested for oxygen impurity, and was found to be at ~1.5%, which is acceptable for the neutron-induced H- and He-production measurements in chromium.

[ANL] Production of a full set of chromium foils was completed.

[ANL] An order was placed with the LANL Chemistry Division for the fabrication of an Np-237 foil for the actinide-capture cross-section measurements.

### **Codes**

[ANL] The first order nodal integral approach for fuel-cycle-method code development has been implemented in a prototypic version of the VARI-ANT code, and the need for high order angular approximations has been verified in several benchmarks that contain low-density nodes.

[ANL] An option was added to the MCNPX code to allow a single collision and escape, enabling direct calculation of double differential cross sections.

[ANL] A number of minor corrections were made to the MCNPX code, including one found by a user in the Netherlands (typo in warning message), netting him a \$20 award.

[ANL] An MCNPX Workshop was held at the M. D. Anderson Medical Center, in Houston, TX, June 16-20.

[ANL] Two MCNPX papers were submitted for publication in the proceedings of the American Nuclear Society AccApp'03 Conference (San Diego, CA): "Neutron Multiplicity Counting for Nuclear Safeguards with MCNPX," and "MCNPX Advances for Accelerator Applications."

### **MALIBU**

[ORNL] The first MALIBU program committee meeting was held in Brussels Belgium at the Belgonucleaire offices. Presentations included an overview of the program, information on the fuel, the measurements, and the expected accuracy of the results. Presentations were also given on MOX-related programs.

[ORNL] The MALIBU schedule calls for the fuel sample to be cut in the next few months and distributed to the laboratories for measurements. The program will be completed in 2005.

[ORNL] The MALIBU participants toured radiochemical laboratories at SCK.CEN in Mol, where some of the isotopic measurements will be performed. A tour of the MOX fuel fabrication facility in near-by Dessel followed the SCK.CEN tour.

[ORNL] Discussions were held regarding contractual matters with the Belgonucleaire sales manager and the MALIBU project manager to discuss options for payment and restrictions on the use of data.

## **STRUCTURAL MATERIALS**

### **LANL Hot-Cell Activities**

[LANL] Following their irradiation in STIP-1, T-91 and SS-316L specimens are being prepared for

## ***Transmutation continued***

hydrogen and helium measurements.

### **Radiation Damage Modeling**

[LANL] The Fe-He MEAM model was presented in an oral session at the ANS AccApp03 meeting in San Diego.

[LANL] Simulations of high-energy cascade on the Fe and Fe-He systems have begun.

### **Materials Handbook**

[LANL] The final version of the Materials Handbook Chapter on Tantalum was completed, and the first formal draft of the Handbook Chapter on HT9 12%Cr Steel was prepared for review.

[PNNL] For the ferritic/martensitic irradiated specimen recovery effort, lists of compact tension specimens and tensile specimens thought to be in storage at PNNL were generated, including their irradiation temperatures range and doses.

[PNNL] The data generation and documentation effort on Soviet ferritic/martensitic alloys irradiated in BN-350 and BOR-60 fast reactors has been extended.

## **COOLANT TECHNOLOGY**

### **DELTA loop**

[LANL] The loop was operated for >5 hrs at temperatures up to 400fC during June. The month's efforts were devoted to reducing the amount of oxygen in the liquid lead-bismuth.

[LANL] A cleaning gas injection line was installed in the melt tank. During installation, oxides were again removed manually from the liquid lead-bismuth's surface and analyzed for composition. Oxygen content had decreased compared to earlier samples.

[LANL] The cleaning gas (6% H<sub>2</sub>/He) was injected into the melt tank for ~300 hrs. LBE was circulated after 30 hrs of H<sub>2</sub>/He injection to check the oxygen sensor readings. One oxygen sensor (located at the hottest point in the loop) malfunctioned, and the other oxygen sensors did not show improvement. Three new oxygen sensors have been fabricated, and a

reusable oxygen sensor design is being developed.

[LANL] We developed an HCP for using oxygen "getters" (such as Mg) in the melt tank. We purchased Mg ribbon, and are investigating possible consequences of using Mg in the loop.

### **LBE Research**

[LANL] The draft US development program plan for LBE technology was submitted to the OECD/NEA LBE Expert Group as a template to prepare an international joint development plan.

[LANL] A DELTA Loop action plan was prepared and submitted to DOE to re-baseline the 1000-hr corrosion test based on the need to develop and test LBE cleanup methods, and clean the LBE of the excess oxides and oxygen for desired coolant chemistry for corrosion testing.

[LANL] An RGA (Residual Gas Analyzer) system was assembled for use in the DELTA Loop to detect cover gas compositions and to monitor potential leaks or changes in coolant chemistry (in addition to oxygen sensors).

[LANL] A correlation between steel-corrosion rates and the loop's thermal-hydraulic parameters has been developed, explicitly demonstrating the non-local nature of corrosion in test loops. This correlation can be easily used to interpret and categorize various test data.

[LANL] Improvements were made to the induction heater and cooling system of the oxygen-sensor calibration stand, involving the procurement and fabrication of a number of components.

## **ACCELERATOR-DRIVEN SYSTEMS** **MUSE**

[ANL] The analysis of dynamic measurements performed during the MUSE4 experiment was revised using reactivities determined by the Modified Source Multiplication (MSM) method.

[ANL] Measurements taken in the SC2 MUSE configuration with the tritium target were completed.



## ***Transmutation continued***

The target will be changed to deuterium in July.

### **MEGAPIE**

[LANL] Review of target drawings and documentation in advance of RFM (Readiness For Manufacturing) continued as the major focus of activity. Most subassemblies were released for manufacture.

[LANL] An internal PSI cost assessment was completed. Deviations from selected vendors were noted, but overall prices were in general agreement, so fabrication can begin.

[LANL] A result of a MEGAPIE Steering Committee Meeting was an agreement to delay start of irradiation until July 2005, following the planned delivery of the target to PSI in May 2004.

[LANL] Other DOE contributions to the MEGAPIE Project included: (1) Review of target drawings and documentation, (2) identification of open issues for some components, and (3) continued work on reliability study. A preliminary "living" reliability assessment document was released.

### **TRADE**

[ANL] The TRADE Target Design Subgroup met twice to finalize a new design of the Ta target that complies with the new requirements for the proton beam (140 MeV proton energy). A new reference design has been produced and is undergoing review.

[ANL] Approvals were granted to transport the miniature fission chambers to Casaccia for use in the TRIGA reactor for TRADE. Also, detectors from Photinis are expected before September; so it appears that all is coming together for an extensive experimental campaign in the fall.

[ANL] MSM (Modified Source Multiplication) method factors were generated at different locations for four different subcritical configurations of TRADE with control rods all inserted as requested by experimentalists. These factors are used for the experimental planning of the subcritical reactivity measurements.

### **UNIVERSITY PROGRAMS**

#### **University of Texas at Austin**

The proliferation resistance assessment methodology was used to produce results for thirteen cases for the Blue Ribbon Committee on Nuclear Nonproliferation. Feedback from the committee, which has been very positive, was used to adjust weighting factors and to improve the methodology. Visual coding and documentation for the methodology and the coding is being completed.

Evaluations of cross-section uncertainty sensitivities were performed for a full-core ADS simulation and a full-core fast reactor simulation using a PVM version of MCNPX linked to ORIGEN and NJOY99, and is now being documented.

#### **University of Florida**

Non-isothermal Thermo-Gravimetric Analysis (TGA) oxidation scans of HT-9 stainless steel were completed.

Data are being compared with the results obtained for the non-isothermal oxidation scan of SS-316L. The weight change per area vs. temperature for SS-316L follows the same trend as HT9 stainless steel from room temperature (RT) to 800°C.

#### **North Carolina State University (NCSTU)**

"Calculations of Radiation Damage at SINQ Target 5" was presented at the ANS AccApp'03 Conference. Two figures of special interest were displayed, containing color-coded contour maps with the structural layout of Target 5 overlaid (layers of the various Pb target rods, specimen rods, and empty rods), correlating the shapes of the color contours with structural and materials features in Target 5. There are some surprises in the contour shapes that are under investigation.

#### **UC Berkeley**

The simplified model for searching for the equilibrium composition of a once-through molten-salt transmuting reactor was improved, reducing the search time by an order of magnitude.

## ***Transmutation continued***

A study of the sensitivity of the molten salt reactor performance to the molten salt feed rate was completed, indicating that criticality can be achieved and an equilibrium actinide concentration can be maintained below the solubility limit over a wide range of feed rates. The fractional transmutation becomes larger with a smaller feed rate. The graphite-to-MS volume ratio giving the peak k-eff is between 2 and 3.

Two papers were submitted for publication in the proceedings of the ANS AccApp'03 Conference (San Diego), "Molten-Salt Type Effect on Once-Through Molten-Salt Transmuters Characteristics," and "Cycle Dependent Fuel Inventory Evolution from ATW Fuel Cycle," and one paper submitted to the ANS GLOBAL'03 (New Orleans), "Reduction of TRU Toxicity in LWR-Spent Fuel by Reference ATW System with LBE-Cooled Subcritical Transmuters."

### **University of Michigan**

We completed a second irradiation of HT-9 and T-91 alloy TEM bars to 3, 7 and 10 dpa at 450°C at He-implanted and non-implanted conditions, which will be used for corrosion measurements in the DELTA loop at LANL.

With active support from Westinghouse Electric Company, effort is underway to develop a global fuel-cycle model for the AP1000 core with the Phenix and ANC codes (to which we have recently been granted full access).

Two papers were submitted for publication in the proceedings of the ANS AccApp'03 Conference (San Diego): "Assessment of Materials for Accelerator Applications using Proton Irradiation," and "Space-Time Correction in Reactivity Determination for Subcritical Systems."

Three papers have been submitted for publication in the proceedings of the ANS GLOBAL'03 Conference (New Orleans): "Transuranics Transmutation Characteristics of Denatured Thorium in Fast Reactors," "Effects of Stockpile Spent Fuel Feed on Recycling Self-Generated Plutonium in PWRs," and

"Evaluation of Different Reactivity Definitions for Subcritical Systems."

### **University of Illinois**

Completed the assembly of a gas system for delivering controlled partial-pressures of oxygen, hydrogen, and water vapor that will provide specific oxidation potentials in an LBE system.

A paper was submitted for publication in the proceedings of the ANS AccApp'03 Conference (San Diego): "The Use of Impedance Spectroscopy to Measure Lead-Bismuth Corrosion."

### **LANLAFCI University Programs Leader**

Two purchase requests for University research projects were submitted to LANL Procurement: one for NCSU to develop an international database (library) of damage cross sections, and another for UC Berkeley to provide input data on impacts of recycling and transmutation on repository performance for LANL systems analyses.

A "Modeling and Measurement of Helium Bubble Effects" project was initiated at UIUC, using a variety of methods to examine effects of He bubble size on properties of steels.

Discussions were held between LANL and NCSU to support LANL's systems modeling efforts, and between LANL and Texas A&M for support of LANL's Gen IV research programs.

The AFCI University Programs Leader ran the technical program of the sixth international topical meeting "Nuclear Applications of Accelerator Technology: AccApp'03," which was imbedded in the ANS summer meeting in San Diego, and has begun a one-year elected position on the Accelerator Applications Division of the American Nuclear Society.

***For more information on Transmutation contact:  
Mike Cappiello (505) 665-6408***

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# University of Nevada LV

## **UNLV Transmutation Research Program (TRP)**

### **Administration**

Prior month's issue was resolved and the payments to the Khlopin Radium Institute were received this month.

UNLV with the support of the TRP successfully recruited an actinide chemistry professor. The tenure-track professor will teach in the Chemistry Department and direct a new actinide laboratory at the Harry Reid Center for Environmental Studies.

The following 13 papers were presented at the American Nuclear Society Conference in San Diego, CA, June 1-5, by UNLV faculty and students:

- M. Holl, M. Trabia, R.A. Schill Jr. (UNLV), "Optimization of a Five Cell Niobium Cavity". (Task 2)
- A.L. Johnson, D. Parsons, J. Manzerova, D.L. Perry, D. Koury, B. Hosterman, and J.W. Farley, "Surface Studies of the Corrosion of Stainless Steel by Lead Bismuth Eutectic: Surface Preparation Effects on 316 Stainless Steels." (Task 3)
- A.K. Roy, R. Prabhakaran, M.K. Hossain, S. Sama, B.J. O'Toole (UNLV), "Environmental-Induced Degradation of Spallation Target Materials." (Task 4)
- C. Wu, K. Dasika, Y. Chen, S. Moujaes (UNLV), J. Zhang, N. Li (LANL), "Study of Geometry Effects on Local Corrosion Rates for LBE Loop". (Task 5)
- D. Curtis (UNLV), D. Beller (LANL), C. Hull (UNLV), A. Rimsky-Korsakov (Khlopin Radium Inst), T. Ward (DOE), "Modeling Neutron Multiplicities in a 60-Element  $^3\text{He}$  Detector System". Undergraduate Dean Curtis received the Best Student Poster Award (Task 6).
- H. Royyuru, L. Sun, Y. Chen, H.-T. Hsieh (Nevada Ctr Adv Comput Meth), R. Clarksean, D.W. Pepper (UNLV), G. Vandegrift, J. Copple, J. Laidler (ANL), "Development of Systems Engineering Model for Spent Fuel Extraction Process". (Task 8)
- M. Lewis, M. Jones, A.K. Roy, B.J. O'Toole

(UNLV), "High-Temperature Deformation of Alloy EP-823 for Transmutation Applications". (Task 10)

- M.A. Reda, J.F. Harmon (Idaho State Univ.), S.B. Sadineni (UNLV), "Properties of Photo-Neutron Sources for Accelerator Driven Sub-Critical Systems". (Task 12)
- M. R. James (LANL), R.T. Klann (ANL), G.L. Morgan, E.J. Pitcher, M.A. Paciotti (LANL), J.M. Oostens (Campbellsville Univ), J.E. Platte (Univ of Michigan), D.R. Lowe (UNLV), "Measurements from Activation Foils of a Proton Irradiated Lead-Bismuth Target". (Task 12)
- X. Wu, R. Sivaraman (UNLV), N. Li, W. Hang, T.W. Darling (LANL), Y. Jiang, W. Yim, B. Fu (UNLV), "Design of an Oxygen Measurement Apparatus for Liquid Lead-Bismuth Eutectic. (Task 13)
- A.K. Roy, V. Marthandam, A. Venkatesh, S.B. Dronavalli (UNLV), "Residual Stress Measurement by Nondestructive and Destructive Methods". (Task 14)
- F.A. Selim, D.P. Wells, J.F. Harmon, J. Kwofie (Idaho State Univ), A.K. Roy (UNLV), "Applications of Electron Linacs in Defect and Stress Measurements." (Task 14)
- A.K. Roy, "Residual Stress Measurements by Nondestructive and Destructive Methods." (Task 14)

### **Issues**

Scope of Work and Work Packages were submitted to DOE for remaining FY03 funding. The UNLV program needs DOE to provide Notice of Financial Assistance Award for the remaining FY03 funding such that accounts can be set up by August 1, 2003.

## **UNLV TRP Student Research**

### **UNLV TRP Fuels**

#### ***Design and Analysis for Melt Casting Metallic Fuel Pins Incorporating Volatile Actinides (Task 1)***

The analysis of mold filling and solidification continues with progress being made for the consideration of these two features within one model.

Analysis of the induction heating process of an Induc-

tion Skull Melter (ISM) continues.

Efforts are underway to validate the modeling procedure and specific comparisons are being made to previously published work. Few detailed modeling results have been reported by other researchers, making the validations an important part of the overall modeling process.

Skin heating depths, power deposition rates, and other process parameters are being evaluated for use in upcoming furnace design simulations.

Efforts are beginning on the development of a numerical model that assesses the impact of americium transport from a heated melt.

## UNLV TRP Separations

### Development of a Systems Engineering Model of the Chemical Separations Process (Task 8)

Efforts have started on the storage of all results in a MS-Access database to speedup and streamline the analysis of multiple runs (parametric studies for design purposes).

An Object Oriented Programming (OOP) approach has been developed and implemented for the final three sections of the new modeling approach (First, Intermediate, and Last sections).

A number of AMUSE analyses were conducted to demonstrate the ability of the code to store the data, plot the data, and to obtain feedback from ANL on how to improve the interface.

The AMUSE code can now be called from within MATLAB as part of the Systems Engineering Modeling effort.

Input files and results files can be successfully generated for individual runs and for multiple runs through MATLAB calls. Refinements will be made to this approach to allow for more runs and to allow for optimization.

### Nuclear Criticality Analyses for Transmuter Fuel Fabrication and Reprocessing (Task 11)

Continuation of summer internship of graduate student Elizabeth Bakker at Argonne National Laboratory.

Continued investigation of criticality tendencies of

mixtures of americium and curium metal.

Continued investigation of criticality tendencies of mixtures of americium oxide and curium oxide.

Performed literature searches for necessary properties of cesium oxide and strontium oxide.

### Immobilization of Fission Iodine by Reaction with a Fullerene-Containing Carbon Compound and Insoluble Natural Organic Matrices (Task 15)

Improved the performance of the iodine generator, by adjusting the size of the nitric acid and iodine chambers. In addition, we have improved temperature control.

Continued experiments with sphagnum moss to study iodide binding. We have conducted experiments at various flow rates to determine breakthrough volumes for the sphagnum columns. With 30% by weight  $\text{Ca}(\text{OH})_2$  break through (concentration exiting column is 5% of inlet) is at ~1000 bed volumes at flow rates of 20-40 mL/min. The iodine concentration was 12 mMol/L and ~50% saturated with nitric acid vapor.

In preparation for FCC testing, we have conducted an iodine breakthrough experiment with carbon nanotubes from Aldrich Chemical. The performance of the carbon nanotube material similar to the peat columns in that break through was at ~1000 bed volumes. However, the rate of break through after 1000 bed volumes was significantly lower than the sphagnum columns.

Examined iodine leaching from sphagnum and carbon nanotubes using colorimetric analysis and ion chromatography. A small quantity of iodide was leachable from the sphagnum. For the carbon nanotubes, a significant amount of sorbed iodine was leachable as molecular iodine.

Calibrating the pyrolysis mass spectrometer for methyl iodide so that the amount of iodide released from iodinated peat as methyl iodide can be quantified.

### Evaluation of Fluorapatite as a Waste-Form Material (Task 16)

Students were trained to work at the soft-x-ray



# University of Nevada LV

Beamline 6.3.1 at the Advanced Light Source (LBNL).

Obtained high resolution XPS spectra for hydroxylapatite (powder) and for fluorapatite (clear and colored crystal as well as the powder).

- Obtained Oxygen K-edge absorption spectra for hydroxylapatite (powder) and fluorapatite (powder).
- Tried to obtain fluorine K-edge spectra for fluorapatite but the signal to noise ratio was too low. Thin film samples will be analyzed to try to improve the signal to noise ratio.
- Prepared hydroxylapatite samples incorporated with Zn (powder) and Mg (grinded as much as possible) in solid phase

## Issues

Task 15 is still awaiting fullerene-containing carbon compounds from Khlopin Radium Institute collaborators.

## UNLV TRP Transmutation Sciences

### Modeling, Fabrication, and Optimization of Niobium Cavities (Task 2)

Track 5.0 (electromagnetic particle tracking program) was employed to study a more realistic sensor geometry as is available on the market.

LEED sensors have been ruled out since they cannot detect single particles.

Anticipate ordering a particle positioning sensor in July.

Attended American Nuclear Society - Accelerator Applications in a Nuclear Renaissance.

- Multipacting data is being analyzed.
- Flow studies are being conducted.
- Flow study thesis is currently being worked on.

### Experimental Investigation of Steel Corrosion in Lead-Bismuth Eutectic: Characterization, Species Identification, and Chemical Reactions (Task 3)

Two undergraduate students, Stacy Sidle (Rhodes College, Memphis TN) and Chris Harland (University of Puget Sound, WA) joined the group in early June. They are funded by the NSF Research Experience

for Undergraduates (REU) grant held by UNLV professors John Farley and Andrew Cornelius. Sidle and Hadley became familiar with the project and the instrumentation and are examining some corroded metal samples using optical microscopes and the SEM.

A third student, Lindsay Wylie, graduated from a Las Vegas area high school in early June, and will enroll at UNLV in the fall as a physics major. She joined the group and helped with the figures for the manuscript for the *Journal of Nuclear Materials*.

Graduate student Brian Hosterman successfully obtained a Raman spectrum from a steel sample exposed to LBE. Previously he had obtained Raman data only from standards. This is an important step forward, and is the first installment of data for his master's thesis.

Design work continued on a proposed very-small-scale experiment in corrosion of steel by LBE.

### Environment-Induced Degradation and Crack-Growth Studies in Candidate Target Materials (Task 4)

Stress corrosion cracking (SCC) testing using self-loaded C-ring and U-bend specimens in acidic solution is ongoing with and without the presence of oxygen. SCC testing in molten LBE using similar types of specimens will soon be initiated at LANL. SCC testing using smooth and notched tensile specimens of Alloys EP-823, HT-9 and 422 in aqueous environments have been initiated.

SCC tests under controlled cathodic potentials (with respect to the corrosion potential) are ongoing to evaluate the effect of hydrogen charging on cracking.

Localized corrosion (pitting and crevice) behavior of all three alloys is being evaluated by cyclic potentiodynamic polarization (CPP) at elevated temperatures.

Metallographic evaluations by optical microscopy and fractographic evaluations by scanning electron microscopy are being continued.



## Modeling Corrosion in Oxygen-Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrogen Transport (Task 5)

“Grid independence” has been determined for our laminar and turbulent flow runs and the researchers have started to make several runs for different flow, and temperature conditions related to the lead-bismuth Delta loop.

## Neutron Multiplicity Measurements of AAA Target/Blanket Materials (Task 6)

Finalized the graphical depiction of the results of nuclear transport models for the neutron production source volume and neutron capture efficiencies of specific elements of the KRI  $^3\text{He}$  60 element detector systems. The target in these models was modified from the AS1 configuration (cylindrical) to rectangular targets. Transport code models of rectangular targets are now being constructed.

$^3\text{He}$  Neutron Multiplicity detector prototype (60 element) is now in transit to UNLV, scheduled to arrive at HRC in mid-July 2003. U.S. Customs was notified of the modified arrival date of KRI detector system in Las Vegas. Arrangements have been made by KRI with a consignment agent at Long Beach, CA where the detector system will be off-loaded. Transport from a bonded warehouse to UNLV will be by truck transport contracted by this customs broker. Costs that accrue from retaining the customs broker will be handled by KRI's consignment agent (all transport costs are being paid by KRI).

The U.S. State Department has issued and modified visas for all three Russian scientists whom are scheduled to install and test the  $^3\text{He}$  detector system during July 26 to August 1, 2003.

The 150 nCi  $^{252}\text{Cf}$  source has been received by the UNLV Radiation Safety Office and will be transferred to the HRC RDL in early July. A shield for this source has been constructed in the source locker and consists of borated paraffin bricks surrounded by lead.

The glass fiber neutron multiplicity detector prototype ( $^6\text{Li}$  glass fiber detector) is approximately 90% complete for all hardware and electronic card production (for optoelectronic interfaces, light guides, signal train, firmware). Cabling and stand-off elec-

tronics shielding has yet to be completed.

## Development of Dose Conversion Coefficients for Radionuclides Produced in Spallation Neutron Sources (Task 7)

Literature search for nuclear data bases for the Category 2 radionuclides continued.

Calculates of DC's completed for the Category 1 radionuclides which have complete ENSDF files.

## Development of a Mechanistic Understanding of High-Temp Deformation of Alloy EP-823 for Transmutation Applications (Task 10)

High-temperature tensile testing using specimen grips made of maraging steel in the presence of nitrogen is in progress. To date, testing has been performed at ambient temperature, 100°C and 300°C.

Future tests involving tensile specimens of Alloy EP-823 will be performed at 400, 500 and 600°C.

Optical microscopy and SEM will be used next to evaluate the metallurgical microstructures and fractography, respectively.

## Radiation Transport Modeling of Beam-Target Experiments (Task 12)

Continued benchmarking on shared memory systems and Beowulf cluster. Testing between MPI versions and PVM. MPI seems to be outperforming PVM by a factor of three on the Beowulf cluster. Runs are currently being conducted on the shared memory systems.

The new machines are AMD 2400's while the older slave machine were AMD 2000's. A program is being made that can look at a cluster and determine the CPU speeds of each computer. Then, the master can determine from this information how large of a job each slave machine should receive.

## Developing a Sensing System for the Measurement of Oxygen Concentrations in Liquid LBE Systems (Task 13)

Two graduate students will be sent to LANL to work on the project after their security clearance has approved by the DOE headquarters.

The assembly of the apparatus has almost been completed. It may be shipped to LANL by the end of the summer.

Some preliminary 3-D simulation results have been obtained for a simplified model.

## ***Use of Positron Annihilation Spectroscopy for Stress-Strain Measurements (Task 14)***

Measurements of residual stresses in welded specimens consisting of similar and dissimilar materials of heat-treated Alloy EP-823 and Type 304L stainless steel by positron annihilation spectroscopy (PAS) are ongoing at the Idaho State University (ISU). PAS data on three-point-bent specimens are currently being analyzed.

Metallographic evaluations of welded specimens are in progress.

A formal proposal has been submitted to the Atomic Energy of Canada Limited (AECL) to perform residual stress measurements in similar materials by using the neutron diffraction technique.

## ***Issues***

The XPS instrument is not working right now because a filament in the argon ion sputtering gun needs to be replaced. The gun was shipped back for repair. (Task 3)

Task 7 is concerned about missing data in the ENSDF files for the radionuclides of interest. While efforts are continuing, the ongoing literature search has not been able to fill all of the holes in the nuclear data bases for radionuclides in the second and third categories. Potential paths to resolve this issue are being discussed, but no path forward has been determined at this time.

***For more information on Transmutation contact:  
Tony Hechanova at 9702) 895-1457.***

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# University Research Alliance - Fellowship Program

## University Programs

FY02 AFCI Fellow Lee Van Duyn, Mechanical Engineering, Georgia Tech, is working at Argonne National Laboratory West this summer. He is working with Steve Hayes, and Mitch Meyer in the Nuclear Technology division. For his master's degree, Lee is working on a project related to the modeling and study of the dispersion of nuclear fuels. He has also been working on further expanding his finite element model, but has been running into a number of computational bugs that have slowed his progress. Other aspects of Lee's model have been coming along, like how to implement creep and fission gas release into the mechanical model. Nearly all the material properties that are needed for the model have been found and are in use. Once the model works satisfactorily, Lee will check it with experimental data available in the literature and decide on a failure criterion that should be able to predict when fuels of this sort will fail. Lee will be back at Georgia Tech on August 17, where he will be taking his final class, finishing up the research and beginning to write his thesis with the intent of graduating in December.

FY02 Fellow Frank Szakaly, Nuclear and Radiological Engineering, Texas A&M University, is spending the summer at Los Alamos National Laboratory where he is working in NMT-11 with Marius Stan, Deborah Bennett, and Bob Margevicius on a Cs/Sr separation project. Frank is also working on finishing up his Master's thesis and is in the middle of running simulations on uranium-free nitride fuels and also series 1 MOX with Np fuels for burning in LWR's. Frank is using MCNP5 and MOCUP/Monteburns to do these simulations.

FY02 Fellow Mike Gregson, Nuclear Engineering, The University of Texas, has graduated and started work at Sandia National Laboratories in the Facilities Support Group. Mike says that he expects to be looking at Ph.D. programs before the year is out.

FY02 Fellow Will Wieselquist, Reactor Physics, North Carolina State, reports that the sensitivity analysis tool that he is developing as part of this master's degree, is now capable of first order perturbation theory of  $k$ , effective for the following types of nuclear data: microscopic absorption cross-section, microscopic fission cross-section, neutrons per fission, and energy released per fission for the U and Pu isotopes. He is currently working on expanding the list of depletable isotopes in NESTLE from just the U-Pu chain and Am-241 to the all important Th, Np, Cm, and Am isotopes. He will soon need to add the capability for Depletion Perturbation Theory (DPT) in order to analyze sensitivity of end-of-cycle isotopics to nuclear data.

Upon graduation with his master's degree, Will hopes to work at Brookhaven National Laboratory where he says he "loved" working during the summer of '02 (following being admitted into the AFCI Fellowship Program).

Management-wise, University Research Alliance is preparing to develop the FY04 Fellowship program. We anticipate that it will include both masters and Ph.D. students.

We are also working on the [studentpipeline.org](http://studentpipeline.org) web site. You may now see a number of the AFCI Fellowship Program graduates' theses on line. We are also developing two new pages: 1) AFCI Fellows – Where are they now?, and 2) The AFCI Fellowship Experience. Both of these pages address the marketing side of the job we were asked to do in administering this program. The AFCI Fellowship Experience will help potential fellowship applicants to visualize the scope of everything students are able to enjoy as AFCI Fellows. It will include colorful photos with cutlines and "pull quotes" which are stand-alone quotes that allow us to emphasize a variety of the different aspects of the program.

Following is a sampling of the most recent quotes we

## ***University Research Alliance - Fellowship Program***

have received from AFCI Fellows:

- "My AFCI fellowship was/is an incredible experience - the generous funding both made my Master's work possible and also gave me the freedom to create a research project of my own choosing, rather than having to follow a professor's work at my graduate school. The experience has been great: meeting with DOE people in Washington as well as my two summers of national lab work at Oak Ridge and Los Alamos, and it even paid for me to attend a couple of helpful and fun conferences!"
- "I'm very grateful I got involved in this program - the opportunity is amazing, and the work schedule while very rigorous, is actually a benefit because it helps provide motivation and direction in a timely fashion to perform our projects. I feel a lot more confident and able to do good quality work since I've started attending graduate school and the AFCI fellowship was a huge part of that."
- "I have been impressed with the level of recognition obtained by AFCI fellows. Letters were written to me from state members of the national Congress congratulating me on my accomplishment as well as being mentioned in my home newspaper." "Being an AFCI fellow allows for increased interaction with members of national laboratories. In my experience this can either come from interactions at conferences or in depth discussions regarding various research topics."
- "I would recommend future students to apply to the AFCI program because of the level of commitment, the technical expertise, and the prestige that I have seen from the program."

***For more information on the University Research Alliance contact: Cathy Dixon at (806) 376-5533***

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## ***Technical Integration***

**[SNL]** Participated in the Engineering Scale Experiment (ESE) 60% Design Review at INEEL and the Transmutation Workshop at ANL.

**[SNL]** Supported HQ in the extensive modification of the program plan to meet NE-1 budget targets and provide documentation for the Office of Management and Budget (OMB) planning document.

**[SNL]** Supported the revision of the Comparison Matrices for the AFCI Report To Congress.

**[SNL]** Hosted the NTD planning meeting in Washington DC on June 23 and 25. At the meeting, the NTDs identified the priorities for FY04 and began to define the deliverables necessary to support a repository recommendation in FY07.

***For more information on Technical Integration  
contact John Kelly: (505) 844-8993***

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